FURTHER CLASSICAL FIFTH-ORDER RUNGE-KUTTA FORMULAS*

H. A. LUTHER†

Introduction

In a previous article [1], three families of classical fifth-order Runge-Kutta formulas were described, and included therein were extensions of Radau, Lobatto, Newton-Cotes and Legendre-Gauss quadratures. It has been possible to improve the approach, so that in this article all previous families, as well as others, are included in a single class of formulas.

Two examples, both of Newton-Cotes type, and neither found in families of [1], are given below

$$y_{n+1} = y_n + \{7k_1 + 7k_3 + 32k_4 + 12k_5 + 32k_6\}/90$$

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf(x_n + h, y_n + k_1)$$

$$k_3 = hf(x_n + h, y_n + \{k_1 + k_2\}/2)$$

$$k_4 = hf(x_n + h/4, y_n + \{14k_1 + 5k_2 - 3k_3\}/64)$$

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†Mathematics Department, Texas A&M University, College Station, Texas

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$$k_5 = hf(x_n + h/2,\ y_n + \{-12k_1 - 12k_2 + 8k_3 + 64k_4\}/96)$$

$$k_6 = hf(x_n + 3h/4,\ y_n + \{-9k_2 + 5k_3 + 16k_4 + 36k_5\}/64).$$

$$y_{n+1} = y_n + \{7k_1 + 12k_3 + 7k_4 + 32k_5 + 32k_6\}/90$$

$$k_1 = hf(x_n,\ y_n)$$

$$k_2 = hf(x_n + h,\ y_n + k_1)$$

$$k_3 = hf(x_n + h/2,\ y_n + \{3k_1 + k_2\}/8)$$

$$k_4 = hf(x_n + h,\ y_n + \{-k_1 - k_2 + 4k_3\}/2)$$

$$k_5 = hf(x_n + h/4,\ y_n + \{4k_1 - 5k_2 + 20k_3 - 3k_4\}/64)$$

$$k_6 = hf(x_n + 3h/4,\ y_n + \{12k_1 + 9k_2 - 12k_3 + 7k_4 + 32k_5\}/64)$$

A third example, of four point Lobatto type, is given next. It, too, is not found in previous families.

$$y_{n+1} = y_n + (k_1 + k_4 + 5k_5 + 5k_6)/12$$

$$k_1 = hf(x_n,\ y_n)$$

$$k_2 = hf(x_n + h,\ y_n + k_1)$$

$$k_3 = hf(x_n + h/2,\ y_n + \{3k_1 + k_2\}/8)$$

$$k_4 = hf(x_n + h,\ y_n + \{-k_1 - k_2 + 4k_3\}/2)$$

$$k_5 = hf(x_n + (5 - \sqrt{5})h/10,\ y_n + \{(25 - 7\sqrt{5})k_1 + (5 - 5\sqrt{5})k_2 + (20 + 4\sqrt{5})k_3 - 2\sqrt{5}\ k_4\}/100)$$

$$k_6 = hf(x_n + (5 + \sqrt{5})h/10,\ y_n + \{(3 + \sqrt{5})k_1 + (1 + \sqrt{5})k_2 + (4 - 4\sqrt{5})k_3 + 2k_4 + 4\sqrt{5}\ k_5\}/20).$$

Still other formulas of Newton-Cotes type, all using the weights 7/90, 7/90, 32/90, 32/90 and 12/90 can be found. A two parameter formula of this type (one not included in the families of [1]) has previously been discovered [3]. A present line of investigation is the comparison of the members of the Newton-Cotes family now known.

Similar remarks hold true for the other types of quadrature mentioned in the first paragraph above. As an instance, we exhibit a three parameter family of Radau type. (In this connection, mention should be made of a class of Radau type, but of implicit character [4].)

$$y_{n+1} = y_n + \{4k_1 + [16 - \sqrt{6} - \lambda]k_3 + [16 + \sqrt{6} - \mu]k_4 + \mu k_5 + \lambda k_6\}/36$$

$$k_1 = hf(x_n,\ y_n)$$

$$k_2 = hf(x_n + \nu h,\ y_n + \nu k_1)$$

$$k_3 = hf\Big(x_n + (6 + \sqrt{6})h/10,\ y_n + \{[(6 + \sqrt{6})10\nu$$
$$- 3(7 + 2\sqrt{6})]k_1 + [3(7 + 2\sqrt{6})]k_2\}/(100\nu)\Big)$$

$$k_4 = hf\Big(x_n + (6 - \sqrt{6})h/10,\ y_n + \{[(-186 + 121\sqrt{6})2\nu$$
$$- (-123 + 78\sqrt{6})]k_1 + [-123 + 78\sqrt{6}]k_2 + [(168 - 73\sqrt{6})4\nu]k_3\}$$
$$/(500\nu)\Big)$$

$$k_5 = hf\Big(x_n + (6 - \sqrt{6})h/10,\ y_n + \{[6(-186 + 121\sqrt{6})\mu\nu$$
$$+ 500(33 - 20\sqrt{6})\nu + 9(41 - 26\sqrt{6})\mu + 1125(-4 + 3\sqrt{6})]k_1$$
$$+ [1125(4 - 3\sqrt{6}) + 9(-41 + 26\sqrt{6})\mu]k_2 + [12(168 - 73\sqrt{6})\mu\nu$$
$$- 2375(9 - 4\sqrt{6})\nu]k_3 + [125(39 + 4\sqrt{6})\nu]k_4\}/(1500\mu\nu)\Big)$$

$$k_6 = hf\Big(x_n + (6 + \sqrt{6})h/10,\ y_n + \{[570(6 + \sqrt{6})\lambda\nu - 57(21 + 6\sqrt{6})\lambda$$
$$- 1900(21 + 4\sqrt{6})\nu + 4275(4 + \sqrt{6})]k_1 + [57(21 + 6\sqrt{6})\lambda$$
$$- 4275(4 + \sqrt{6})]k_2 + [475(39 - 4\sqrt{6})\nu]k_3 + [2375(9 + 4\sqrt{6})\nu$$
$$- 60(48 + 17\sqrt{6})\mu\nu]k_4 + [60(48 + 17\sqrt{6})\mu\nu]k_5\}/(5700\lambda\nu)\Big).$$

<u>The New Sufficient Conditions</u>

The differential system considered is of course $\frac{dy}{dx} = f(x, y)$ together with $y(x_0) = y_0$. The fifth-order Runge-Kutta formulas are phrased as

$$y_{n+1} = y_n + \sum_{i=1}^{6} R_i k_i$$

$$k_1 = hf(x_n, y_n)$$

$$k_s = hf(x_n + a_s h, y_n + \sum_{j=1}^{s-1} b_{sj} k_j$$

where $2 \leq s \leq 6$.

The sufficient conditions are

(1) $R_2 = 0.$

(2) $a_2 \neq 0.$

(3) $a_i \neq 0,\ a_i \neq a_j$ if $i \neq j,\ 3 \leq i, j \leq 6.$

(4) $(a_6 - 1)(a_3 - 2a_4 + 8a_3a_4 - 10a_3^2 a_4) = 0.$

(5) $$a_3(a_3 - a_4)(a_3 - a_5)(a_3 - a_6)R_3 = \frac{1}{5} - \frac{1}{4}(a_4 + a_5 + a_6) + \frac{1}{3}(a_4a_5 + a_5a_6 + a_6a_4) - \frac{1}{2} a_4a_5a_6$$

$$a_4(a_4 - a_3)(a_4 - a_5)(a_4 - a_6)R_4 = \frac{1}{5} - \frac{1}{4}(a_3 + a_5 + a_6) + \frac{1}{3}(a_3a_5 + a_5a_6 + a_6a_3) - \frac{1}{2} a_3a_5a_6$$

$$a_5(a_5 - a_3)(a_5 - a_4)(a_5 - a_6)R_5 = \frac{1}{5} - \frac{1}{4}(a_3 + a_4 + a_6) + \frac{1}{3}(a_3a_4 + a_4a_6 + a_6a_3) - \frac{1}{2}a_3a_4a_6$$

$$a_6(a_6 - a_3)(a_6 - a_4)(a_6 - a_5)R_6 = \frac{1}{5} - \frac{1}{4}(a_3 + a_4 + a_5) + \frac{1}{3}(a_3a_4 + a_4a_5 + a_5a_3) - \frac{1}{2}a_3a_4a_5.$$

(6) $$R_1 + R_2 + R_3 + R_4 + R_5 + R_6 = 1.$$

(7) $$a_5(a_5 - a_3)(a_5 - a_4)b_{65}R_6 = \frac{1}{20} - \frac{1}{12}(a_3 + a_4) + \frac{1}{6}a_3a_4$$

$$a_4(a_4 - a_3)(a_6 - a_5)b_{54}R_5 = -\frac{1}{15} + \frac{1}{12}a_6 + \frac{1}{8}a_3 - \frac{1}{6}a_3a_6$$

$$a_4(a_4 - a_3)(a_5 - a_4)(b_{54}R_5 + b_{64}R_6) = -\frac{1}{20} + \frac{1}{12}(a_3 + a_5) - \frac{1}{6}a_3a_5.$$

(8) $$R_6\{(a_4 + a_6 - 2a_5)R_4R_6b_{65} + (a_5 - a_6)(b_{54}R_5 + b_{64}R_6)R_5\} \neq 0 \text{ if } a_6 \neq 1.$$

(9) $$a_3b_{43}R_4 + a_3b_{53}R_5 + a_3b_{63}R_6 = \frac{1}{6} - a_4(b_{54}R_5 + b_{64}R_6) - a_5b_{65}R_6$$

$$a_3(a_4 - a_3)b_{43}(b_{54}R_5 + b_{64}R_6) + a_3(a_4 - a_3)b_{53}b_{65}R_6 = -\frac{1}{60} + \frac{1}{24}a_4$$

$$a_3(a_4 - a_5)b_{43}R_4 + (a_6 - a_5)a_3b_{63}R_6 = \frac{1}{8} - \frac{1}{6}a_5 + (a_5 - a_6)(a_4b_{64} + a_5b_{65})R_6.$$

(10) $$\sum_{j=2}^{s-1} a_jb_{sj} = \frac{1}{2}a_s^2, \quad 3 \leq s \leq 6.$$

$$(11)\quad \sum_{j=1}^{s-1} b_{sj} = a_s, \quad 2 \leq s \leq 6.$$

Except that a_2 may not be zero, it is completely a parameter. When a_3, a_4, a_5 and a_6 have been chosen in accordance with (3) and (4), R_3, R_4, R_5, R_6 can be found from (5). Then $b_{65}R_6$, $b_{54}R_5$ and $(b_{54}R_5 + b_{64}R_6)$ follow from (7). It is known [2] that R_6 may not be zero (this is reflected in (8)). If $R_5 = 0$, b_{54} is a parameter. In any event, b_{64} then follows.

The negative condition of (8) is sufficient to allow (9) to be solved for $b_{43}R_4$, $b_{53}R_5$ and $b_{63}R_6$. From this follow permissible values of b_{43}, b_{53}, b_{63}. When $a_6 = 1$, the equations of (9) are linearly dependent and two parameter families may be found.

Then b_{32}, b_{42}, b_{52}, b_{62} follow from (10) and b_{31}, b_{41}, b_{51}, b_{61} from (11). The Radau family listed violates (3). Its validity can be established by direct substitution in relations (5), (7), (8), (9) of the previous article [1].

Derivation of the Conditions

The nomenclature employed is that of [1], and sufficient conditions will be taken therefrom. Of the relations above (1), (5), (6), (10) and (11) are essentially relations (7), (9b), (9a), (8), and (5) in [1]. The only variation involves (5) above, which is equivalent to (9b) in [1] in view of relation (3) above.

Relation (2) guarantees that (10) is useable.

It remains to show that (4), (7) and (9) are in essence tantamount to relations (9c) and (9d) of [1]. For ease in presentation, these are reproduced below with new numbering.

(12a) $a_3b_{43}R_4 + (a_3b_{53} + a_4b_{54})R_5 + (a_3b_{63} + a_4b_{64} + a_5b_{65})R_6 = \frac{1}{6}$

(12b) $a_3{}^2b_{43}R_4 + (a_3{}^2b_{53} + a_4{}^2b_{54})R_5 + (a_3{}^2b_{63} + a_4{}^2b_{64} + a_5{}^2b_{65})R_6 = \frac{1}{12}$

(12c) $a_3{}^3b_{43}R_4 + (a_3{}^3b_{53} + a_4{}^3b_{54})R_5 + (a_3{}^3b_{63} + a_4{}^3b_{64} + a_5{}^3b_{65})R_6 = \frac{1}{20}$

(12d) $a_4a_3\,b_{43}R_4 + a_5(a_3b_{53} + a_4b_{54})R_5 + a_6(a_3b_{63} + a_4b_{64} + a_5b_{65})R_6 = \frac{1}{8}$

(12e) $a_4a_3{}^2b_{43}R_4 + a_5(a_3{}^2b_{53} + a_4{}^2b_{54})R_5 + a_6(a_3{}^2b_{63} + a_4{}^2b_{64} + a_5{}^2b_{65})R_6 = \frac{1}{15}$

(12f) $a_3b_{43}b_{54}R_5 + [a_3b_{43}b_{64} + (a_3b_{53} + a_4b_{54})b_{65}]R_6 = \frac{1}{24}$

(12g) $a_3{}^2b_{43}b_{54}R_5 + [a_3{}^2b_{43}b_{64} + (a_3{}^2b_{53} + a_4{}^2b_{54})b_{65}]R_6 = \frac{1}{60}$

The first equation of (9) is (12a).

The third equation of (9) is (12d), minus a_5 times (12a).

The second equation of (9) is a_4 times (12f), minus (12g).

The first equation of (7) is (12d) minus a_3 times (12e), minus a_4 times (12b), plus a_3a_4 times (12a).

The third equation of (7) is $(a_5 - a_4)$ times (12b), minus $a_3(a_5 - a_4)$ times (12a), together with use of the first of (7).

The second equation of (7) is a_6 times (12b), minus a_3a_6 times (12a), minus (12e) plus a_3 times (12d).

Finally, relation (4) is a consequence of (12g) minus a_3 times (12f), together with the first two equations of (7) and the third of (5).

The requirement (3) guarantees equivalence. Requirement (8) is added to guarantee solution of (9) for b_{43}, b_{53}, b_{63}.

References

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4. ____________ , Integration Processes Based on Radau Quadrature Formulas, Math. Comp., 18(1964), pp. 233 - 244.